

=>

Uploading C:\Program Files\Stnexp\Queries\10580610-casreact.str



ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-7 8-9 8-13 9-10 10-11 11-12 12-13 12-14

13-16 14-15 15-16

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-7 8-9 8-13 9-10 10-11 11-12 12-13 12-14

13-16 14-15 15-16

isolated ring systems :

containing 1 : 8 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom

fragments assigned product role:

containing 8

fragments assigned reactant/reagent role:

containing 1

node mappings:

3:10 4:11 2:9 1:8 6:13 5:12

L13 STRUCTURE UPLOADED

=> s l13 sss full

FULL SEARCH INITIATED 09:16:27 FILE 'CASREACT'

SCREENING COMPLETE - 2556 REACTIONS TO VERIFY FROM 244 DOCUMENTS

100.0% DONE 2556 VERIFIED 29 HIT RXNS 9 DOCS

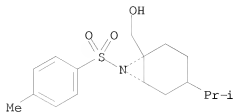
SEARCH TIME: 00.00.01

L15 9 SEA SSS FUL L13 ( 29 REACTIONS)

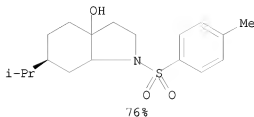
=> d l15 tot

L15 ANSWER 1 OF 9 CASREACT COPYRIGHT 2008 ACS on STN

RX(209) OF 518 - 2 STEPS



1. NaH, THF
2. Corey's reagent,  $\xrightarrow{\text{DMSO}}$



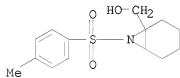
REF: Journal of the American Chemical Society, 129(7), 1996-2003; 2007

NOTE: 1) regioselective

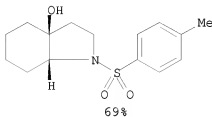
CON: STEP(1.1) 4 hours, room temperature; room temperature  $\rightarrow$  0 deg C  
STEP(2.1) room temperature  $\rightarrow$  85 deg C; 24 hours, 85 deg C

L15 ANSWER 2 OF 9 CASREACT COPYRIGHT 2008 ACS on STN

RX(31) OF 38 - 2 STEPS



- 1.1. KH, THF
- 1.2. NH4Cl, Water
- 2.1.  $\text{Me}_3\text{SO}, \text{I}, \text{BuLi}, \xrightarrow{\text{THF, Hexane}}$
- 2.2. DMPU, THF
- 2.3. NH4Cl, Water



REF: Chemical Communications (Cambridge, United Kingdom), (30), 3226-3228; 2006

CON: STEP(1.1) -78 deg C; 5 minutes, -78 deg C  $\rightarrow$  0 deg C;  
120 minutes, 0 deg C

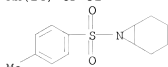
STEP(1.2) 0 deg C

STEP(2.1) 15 minutes, -78 deg C; 15 minutes, 0 deg C

STEP(2.2) -78 deg C; 5 minutes, -78 deg C  $\rightarrow$  room temperature;  
120 minutes, reflux

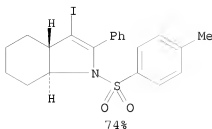
L15 ANSWER 3 OF 9 CASREACT COPYRIGHT 2008 ACS on STN

RX(24) OF 32



(step 1)

1. Phenylacetylene,  
NaH, DMSO
2. I2, AgOAc
3. Na2S2O3, Water



74%

REF: Tetrahedron, 61(40), 9586-9593; 2005

NOTE: molecular sieves used in stage 1, alternative preparation increased yield

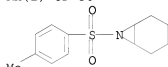
CON: STAGE(1) 2 hours, room temperature

STAGE(2) room temperature -> 40 deg C; 5 hours, room temperature

STAGE(3) room temperature

L15 ANSWER 4 OF 9 CASREACT COPYRIGHT 2008 ACS on STN

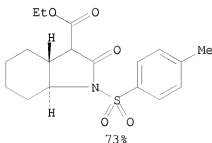
RX(2) OF 36



(step 2)



1. NaOEt, THF



73%

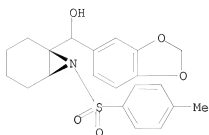
REF: PCT Int. Appl., 2005054194, 16 Jun 2005

CON: STAGE(1) 0.75 hours, reflux

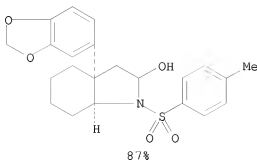
STAGE(2) 1 hour, reflux; 15 hours, reflux

L15 ANSWER 5 OF 9 CASREACT COPYRIGHT 2008 ACS on STN

RX(41) OF 133 - 3 STEPS



- 1.1.  $\text{ZnBr}_2$ ,  $\text{CH}_2\text{Cl}_2$
- 1.2. Water
- 2.1.  $\text{Ph}_3\text{PCH}_2\text{OMe} \cdot \text{Cl}$ , THF
- 2.2.  $\text{BuLi}$ , Hexane  $\rightarrow$
- 2.3. THF
- 2.4. Water
- 3.1.  $\text{HClO}_4$ ,  $\text{Et}_2\text{O}$ , Water
- 3.2.  $\text{NaHCO}_3$ , Water



REF: Organic Letters, 5(13), 2319-2321; 2003

NOTE: 1) key step, stereoselective, 2) 1:1 E:Z

CON: STEP(1) 1 hour, room temperature

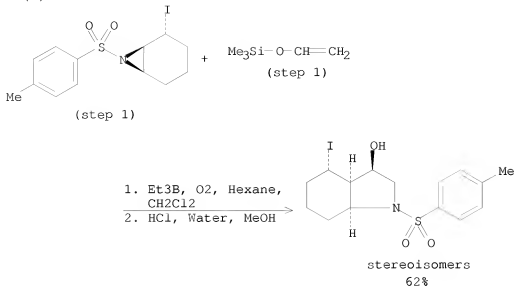
STEP(2.1) room temperature  $\rightarrow$  0 deg C

STEP(2.2) 1 hour, room temperature

STEP(2.3) 0 deg C; 0.5 hours, room temperature

STEP(3.1) 8 hours, room temperature; room temperature  $\rightarrow$  0 deg C

RX(7) OF 24



REF: Journal of Organic Chemistry, 68(8), 3184-3189; 2003

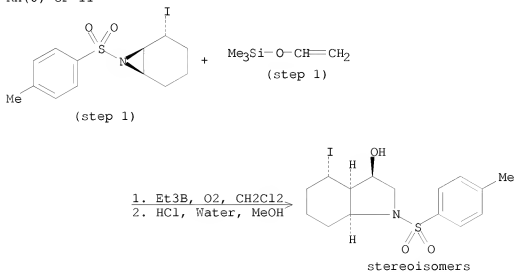
NOTE: stereoselective

CON: STAGE(1) 10 hours, room temperature

STAGE(2) 2 hours, room temperature

L15 ANSWER 7 OF 9 CASREACT COPYRIGHT 2008 ACS on STN

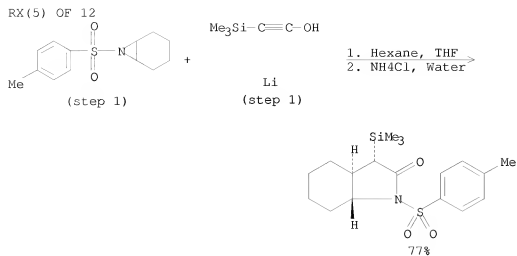
RX(8) OF 11



REF: Angewandte Chemie, International Edition, 40(20), 3865-3867; 2001

NOTE: <62>% overall yield

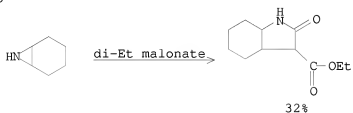
L15 ANSWER 8 OF 9 CASREACT COPYRIGHT 2008 ACS on STN



REF: Journal of Organic Chemistry, 66(1), 169-174; 2001  
NOTE: stereoselective

L15 ANSWER 9 OF 9 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 6



REF: Yakugaku Zasshi, 95(7), 889-92; 1975